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Electrical Resistivity/ Resistance of Cu Doped As-Se glasses

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ABSTRACT

The theoretical calculation for pressure dependence of electrical resistance has been carried out for Cu Doped As-Se glasses. The calculated results for the $Cu_xAs_{40}Se_{60-x}$ glasses with x between 0 and 28% show that the resistivity of glasses continuously decreases and saturates at higher quasi-hydrostatic pressures. The results have been compared with the experimental data and yield a good description of variation of electrical resistivity with pressure.

Key Words: Resistance, Cu Doped As-Se glasses, $Cu_xAs_{40}Se_{60-x}$ glasses.

INTRODUCTION

Generally, As-Se glasses are lone pair semiconductors in P-type conduction. The Fermi level in chalcogenide glasses is pinned near the midgap as the added impurities enter the material in an alloying sense as a result doping is not possible [1]. There are some exceptions that bismuth/lead doped Ge-Se (S, Te) glasses are found to exhibit n-type conduction at critical concentration of Bi/Pb [2,3]. In amorphous tetrahedral semiconductor (Such as a-Si:H) the Fermi level can be moved away from midgap towards one of the band edges by doping. Thus a possible way of doping chalcogenide glasses might involve increasing the coordination number of the chalcogen atoms to four [4]. Under high pressures lone-pair semiconductor glasses exhibit semiconductor-metal transition with a continuous decrease in resistivity [5,6]. On the other hand, tetrahedrally bonded glassy semiconductor (a-Si and a-Ge-type) undergoes a discontinuous transition with changes in structure to high coordination [7]. Cu-As-Se glasses received wide attention due to the possibility of tailoring their electronic band structure from that of a lone pair semiconductor to a tetrahedral semiconductor by varying the concentration of Cu. In Cu-As-Se glasses for all compositions, the coordination of Cu is found to be four and for Cu to be in four fold co-ordination, formal transfer of lone pair electrons from Se or As atoms must take place. This results in the changes in local structure around each atom [8].

Formula Used for Calculations:
The calculations in the present work are based on the following formula [9].

$$R(P) = A(P/Pc)^{\alpha}e^{-\beta}(P/Pc) \quad (1)$$

Where R(P) denotes the resistance of a given solid at pressure P. A, α and β are adjustable parameters and Pc is an arbitrary pressure for making β dimensionless. Equation (1) may also be written in the logarithmic form as given below:

$$\log R(P) = \log A + \alpha \log(P/Pc) - \beta(P/Pc) \quad (2)$$

Since the influence of compression on the dimensions of the solid is small, one can write a similar equation for resistivity ρ in a form similar to Equation (1) as

$$\rho = A_0(P/Pc)^{\alpha}e^{-\beta}(P/Pc) \quad (3)$$

$$\log \rho = \log A_0 + \alpha \log(P/Pc) - \beta(P/Pc) \quad (4)$$

For the sake of the comparison, the pressure coefficient of logarithm of resistivity has been also calculated here. This coefficient may be calculated from the equation (4) is written as

$$\frac{d \log \rho}{dP} = \frac{\alpha}{P} - \frac{\beta}{Pc} \quad (5)$$

In this paper, the resistance/resistivity calculations have been made for a number of materials. For each of the materials, the analysis has been carried out with the help of the Equations (1-4) and the results are compared with the available experimental data. The deviations between theory and experiment have been estimated with the help of a quantity:

$$S = \sum_{i=1}^{n}[\{\text{Experimental value}\}_i - \{\text{Theoretical value}\}_i]^2 \quad (6)$$

Depending on the nature of the data available, the experimental or theoretical value in Equation (6) will correspond to either resistance or resistivity or some other related physical quantity. In the above equation n stands for the number of total pressures considered in the calculations. The parameters A, α and β are varied in such a manner so as to make S minimum. This ensures a best possible agreement between the theory and the experiment.

Theory:

According to this formulation, the resistance to the flow of electrons in a solid at high pressure may be determined by the following relation.

$$\frac{R_P}{R_0} = A(\frac{P}{Pc})^{\alpha}\exp(-\beta\frac{P}{Pc}) \quad (7)$$

Here R_0 and R_p are the resistances of a semiconductor at ambient and high pressure P, respectively A, α and β are the parameters having values depending on the nature of the semiconductor, P_c is an arbitrary pressure introduced to make β dimensionless. The details of this formulation are underlined in Reference [9]. However, for the sake of completeness; we wish to mention some of its features in the present work also. The resistance R_p of a semiconductor may be written in the form of a following polynomial of pressure P[73]

$$R_P = a_0P + a_1P^2 + a_2P^3 + \cdots$$
$$R_P = a_0P(1 + b_1P + b_2P^2 + \cdots) \quad (8)$$

Where $b_j = a_j / a_0$ with j = 1, 2, 3…

When pressure is applied on semiconductor, it results in the overlap of charge distribution of two nearest atoms/molecules which will make a repulsive contribution to the interaction energy of two atoms/molecules. Several empirical forms describing this repulsive interaction are available in literature. According to M.P. Tosi [10], the repulsive interaction between two atoms may have the exponential form $e^{-d/B}$ where d is intermolecular co-ordinate and B is the measure of the range of the interaction. At high pressure, d will be function of P. In view of this, the quantity in bracket has been approximated by an exponential term $e^{-\beta P}$. On account of this, the equation (8) is unbalanced and this imbalance has been somewhat adjusted by putting a power of α on P. The resulting equation (7), thus, incorporates both the assumptions of Drickamer in phenomenological manner and is found to give a reasonable description of pressure induced resistance of a semiconductor.

Calculations:

The effect of pressure on electrical resistivity of $Cu_xAs_{40}Se_{60-x}$ glasses, were experimentally investigated by K. Ramesh [11], carried out at room temperature in a Bridgman anvil system with Pyrophillite as the gasket and steatite as the quasi-hydrostatic pressure transmitting medium. From these results one can easily extract information about the variation in electrical resistivity of these semiconductors against pressure by using the value of linear compressibility $\beta_0(\approx 3\times10^{-4}$kbar). The theoretical calculation for pressure dependence of electrical resistance has been carried out by changing the value of the parameters A, α and β appearing in equation (16) in such a manner so as to obtain a least square fit with the measured data.

The calculated result for the $Cu_xAs_{40}Se_{60-x}$ glasses with x between 0 and 28% show that the resistivity of glasses continuously decreases and saturates at higher quasi-hydrostatic pressures. The results have been compared with the experimental data in figures 1-7, respectively for the $Cu_xAs_{40}Se_{60-x}$ glasses with x between 0 to 28%. It is clear that equation (16) yield a good description of variation of electrical resistivity with pressure. The values of the parameters used in the calculations are quoted in tables 1-7.

Table 1: Values of the Parameters used for calculation X=0

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity Calculation	$\log_e A = 3.4505$	$\alpha = 1.4557$	$\beta = 6.2600$

Table 2: Values of the Parameters used for calculation X=5

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity Calculation	$\log_e A = 1.3883$	$\alpha = 0.6431$	$\beta = 3.6067$

Table 3: Values of the Parameters used for calculation X=10

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity Calculation	$\log_e A = -3.5754$	$\alpha = -1.9689$	$\beta = 0.4212$

Table 4: Values of the Parameters used for calculation X=15

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity Calculation	$\log_e A = -3.1691$	$\alpha = -1.6024$	$\beta = 0.6968$

Table 5: Values of the Parameters used for calculation X=20

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity Calculation	$\log_e A = -2.3141$	$\alpha = -1.4229$	$\beta = 0.5391$

Table 6: Values of the Parameters used for calculation X=25

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity calculation	$\log_e A = -2.6408$	$\alpha = -1.7936$	$\beta = 0.1231$

Table 7: Values of the Parameters used for calculation X=28

Material Cu-doped As-Se glasses	Values of the Parameters		
Resistivity calculation	$\log_e A = -3.1441$	$\alpha = -2.0327$	$\beta = 0.628$

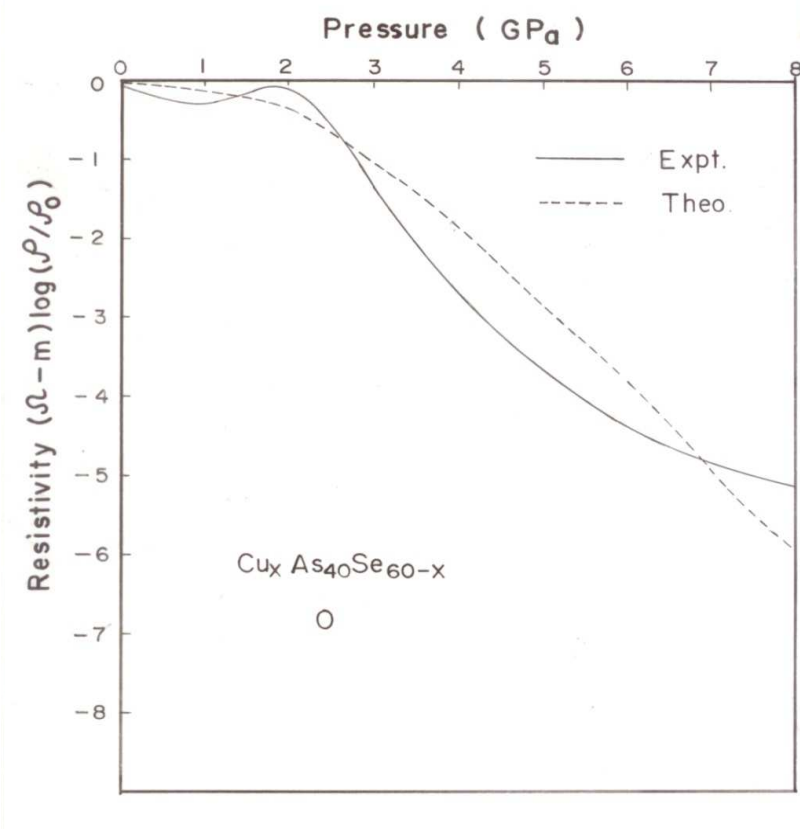

Figure 1: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 0

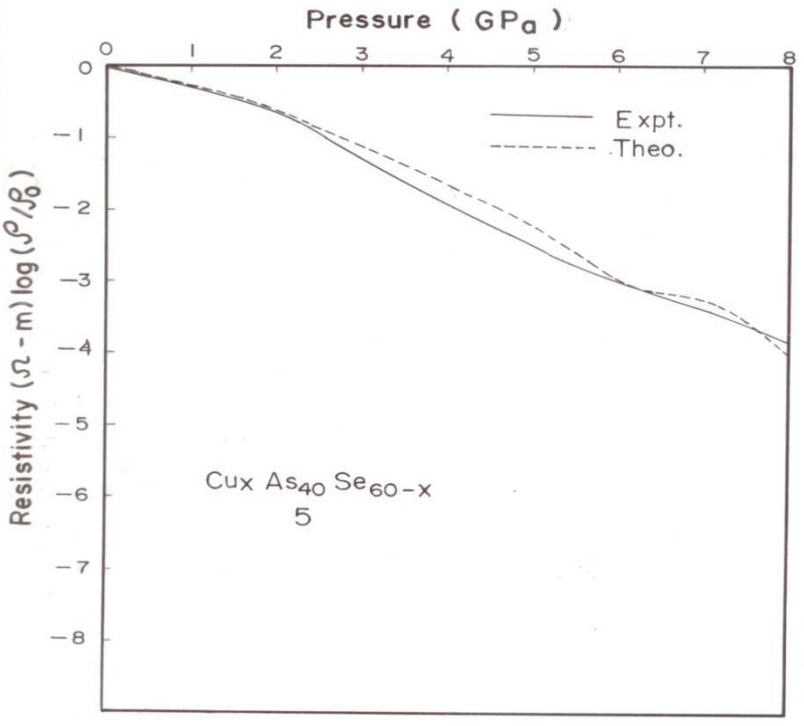

Figure 2: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 5

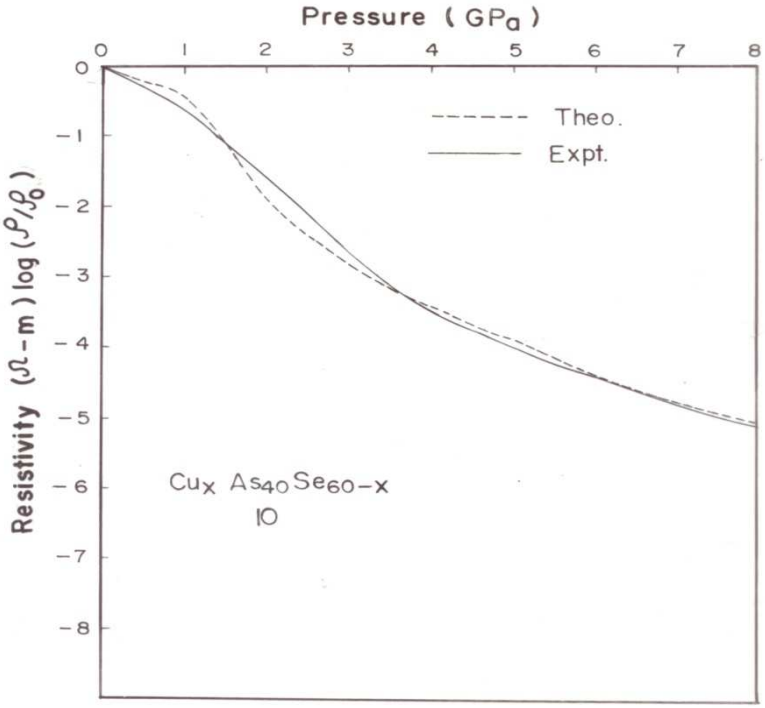

Figure 3: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 10

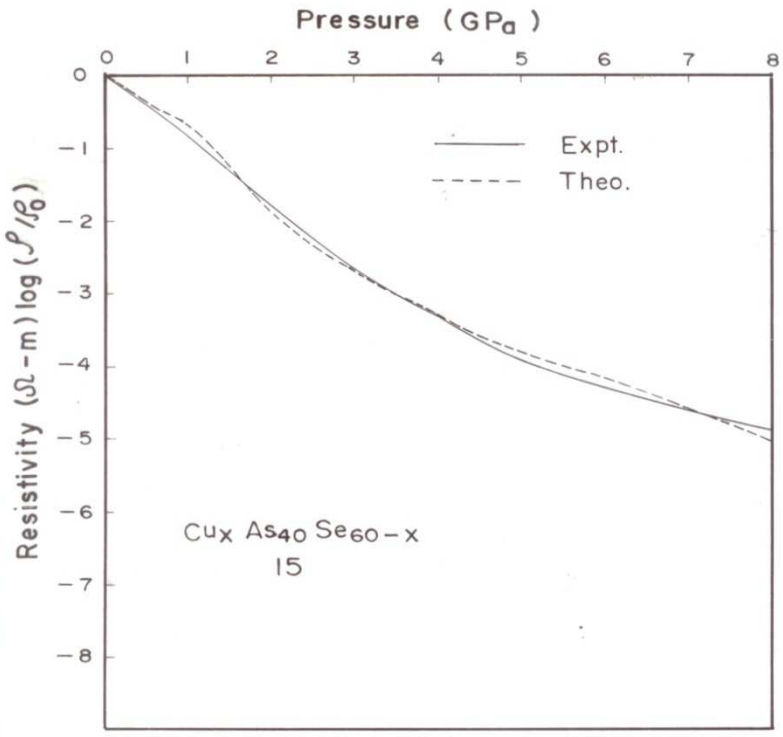

Figure 4: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 15

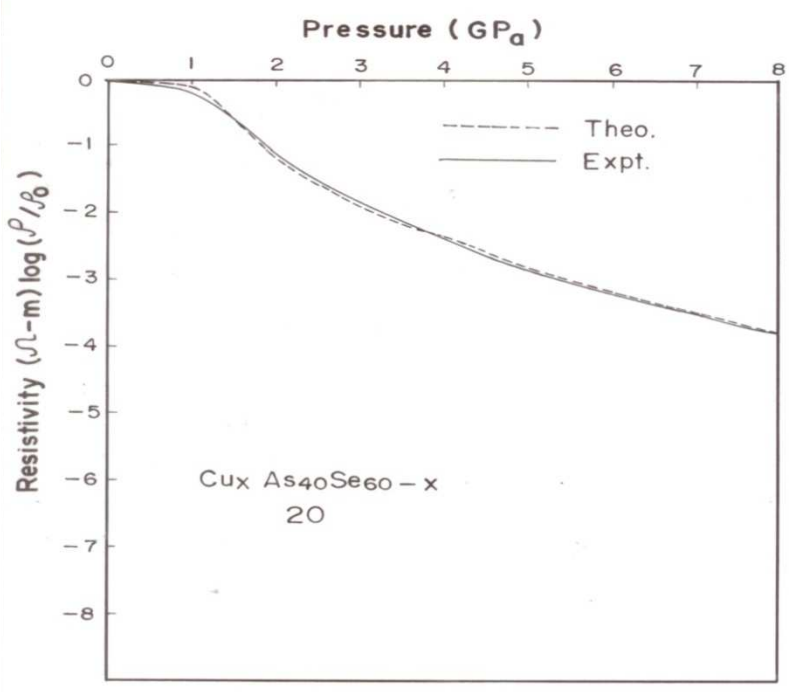

Figure 5: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 20

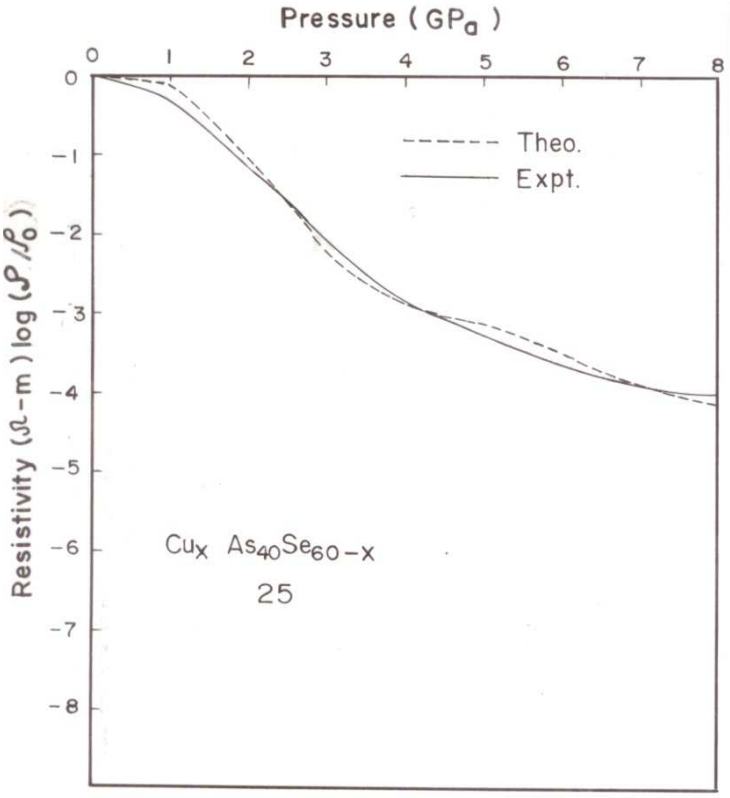

Figure 6: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 25

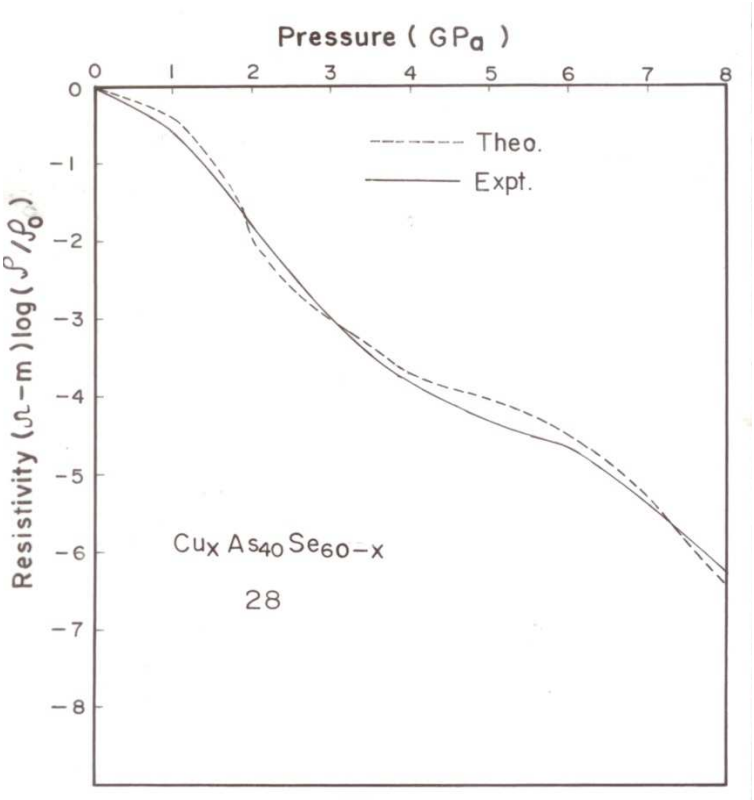

Figure 7: Electrical Resistivity of Cu_XAs_{40} Se_{60-X} glasses as a function of Composition with x = 28

DISCUSSION

A comparison of the present calculation with the experimental results [11] show that the deviation of theoretical value from the measurement is on variation of normalized electrical resistivity of $Cu_xAs_{40}Se_{60-x}$ glasses as a function of pressure. It can be seen that the resistivity continuously decreases with pressure and saturates at high pressures. Upon releasing the pressure the resistivity of all these samples is found to be reversible. The glasses with X = 0 and X = 5 show only small changes in the resistivity at pressures ≤ 1.4 GPa. However, at intermediate pressures 1.4 ≤ p ≤ 5 GPa, the decrease in resistivity tends to saturate. The pressure derivative of electrical resistivity of $Cu_xAs_{40}Se_{60-x}$glasses at different pressures shows distinct change as a function of copper content figures 1-7. The pressure derivative shows steep decrease for the initial addition of Cu with minimum at x=10 and it saturates for the higher content of Cu in the pressure range ≤ 2 GPa for higher pressure (2.5 and 3 GPa) the derivative initially increases and saturates for ≥ 10 at % to Cu. The interesting result of the present work is the composition dependence of the pressure derivative of electrical resistivity and the thermal crystallization. The composition dependence of pressure derivative for lower pressures (≤ 2 GPa) (i) 0 ≤ x ≤ 10 with steep decrease, region (ii) x = 15 and 20 with small increase (iii) 25 and 28 with a tendency to saturate.

CONCLUSION

Under pressure the different structural units (As_2Se_3, Cu_3AsSe_4 and Cu_2 As_3) present in the $Cu_xAs_{40}Se_{60-x}$ glasses as a function of Cu, may differ in compressibilities. In addition, the ratio of these structural units also varies with the composition. Higher compressibility may correspond to a higher pressure coefficient of resistivity. In this way, As_2Se_3 may have higher compressibility compared to Cu_3AsSe_4 and Cu_2As_3 species. Correspondingly the presence of As_2Se_3 in the region (i) 0≤x≤10 probably results in the larger pressure coefficient of resistivity in the pressures range up to 2.0 GPa.

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